Title: Nuclear Data Evaluation Highlights

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Nuclear Data Evaluation

Highlights

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Theoretical division, T-2

2022 MCNP® User Symposium
## Materials & reactions of interest

### Overview & Motivation

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<th>Reactions</th>
<th>Applications</th>
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<td><strong>Actinides</strong></td>
<td>– Stockpile stewardship [weapons]</td>
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<tr>
<td>– ((n,\gamma)): DANCE</td>
<td>– Criticality safety [reactors]</td>
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<tr>
<td>– ((n,\beta)): DANCE/chi-nu/SPIDER</td>
<td>– Basic science [nuc-astro (r-process)]</td>
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<td>– ((g,x))</td>
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<td><strong>Medium mass</strong></td>
<td>– Nuclear energy</td>
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<td>– (^{58}\text{Ni}): LNZ</td>
<td>– Structural materials</td>
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<td>– (^{35}\text{Cl}(n,p)): LNZ</td>
<td>– Diagnostics</td>
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<td><strong>Light elements</strong></td>
<td>– Stockpile stewardship</td>
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<tr>
<td>– (^{12,13}\text{C}(n,z) &amp; (^{16}\text{O}(n,z)): LNZ</td>
<td>– Structural materials &amp; Diagnostics</td>
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<td>– (^{6}\text{Li}(n,z)): NZ</td>
<td>– Fusion energy/basic science</td>
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State-of-the-art Theoretical Modeling

Model & evaluation approaches; LANL codes

- **CoH₃**: Coupled-channels & Hauser-Feshbach code
  - Optical models; compound reaction; pre-equilibrium; direct capture; FRDM mean-field + Hartree-Fock

- **CGMF**: Cascading Gamma-ray Multiplicity for Fission
  - Monte Carlo Hauser-Feshbach statistical theory
    - Emitted-particles correlation; average properties
    - PFNS, $\bar{\nu}$, gamma multiplicity $M_\gamma$, etc.

- **BeoH**: Deterministic implementation of CGMF
  - Delayed quantities, cumulative yields, photofission (new)

- **LISE**: Time-dependent density functional theory
  - HPC TDDFT for superfluid nuclei; Average FF properties

- **EDA₉₀**: relativistic multichannel unitary R-matrix

- Machine Learning/Quantum computing
  - ML: Mixture Density Networks for FF uncertainty quantification
  - QC: Exploratory applications to nuclear shell model

LISE simulation of the time evolution of the fissioning nucleus from a compact shape to two separated fragments. The neutron density is shown at an instance of almost full separation.

$E_D_{90}$ deuteron elastic differential cross section
CGMF and BeoH consistently calculate prompt/delayed fission observables

CGMF and BeoH both begin with equivalent initial conditions for the fission fragments, so delayed observables calculated with BeoH can be connected back to prompt correlations from CGMF.

CGMF exactly takes into account multi-chance fission (Monte Carlo).

BeoH accurately calculates small yields to the same accuracy as large yields (deterministic).
Chi-Nu data & CGMF evaluation

Data Is Used to Improve $^{239}$Pu evaluations

- A CEA collaboration used Chi-Nu to measure very precise $\nu$ data which was combined with CGMF modeling for a recent evaluation.
- LANL Chi-Nu PFNS measurements extended the range of incident and outgoing neutron energies for improved evaluations.
- Combined - with an updated (n,f) cross section evaluation – changes to fission observables perform well in critical assembly benchmarks.

CGMF modeling has been used to evaluate $\bar{\nu}$ for the first time. PFNS evaluation using the Los Alamos model. Evaluations performed by D. Neudecker (LANL/XCP-5)
CoH/BeoH Extended to Photon-Induced Multi-Chance Fission

Photo-nuclear reaction on $^{235}\text{U}$, $^{238}\text{U}$, and $^{239}\text{Pu}$ calculated based on the BeoH model parameters obtained by Shin Okumura for the neutron-induced fission calculations [JNST 59, 96 (2022)]
Photofission product yields (preliminary)

No fit to the data (default parameters)
**181Ta evaluation**

Consistent, model based (EMPIRE) evaluation reproducing selected differential data and well performing in integral testing

Tex (new experiment) - essential improvement compared to ENDF/B-VIII.0 and JENDL-5.0

Further amelioration possible with the new $^{239}\text{Pu}$

- 1st inelastic - major difference to JENDL5 driven by modeling consistency
- Capture - model forced to follow selected experimental data

![Graphs showing cross-sections and energy data for 181Ta](image-url)
Medium mass evaluations
LANL CoH3 Hauser-Feshbach code

Recent measurements

- **Chlorine:** $^{35}\text{Cl}(n,p)$
  - calculation performed for *PRC102, 024623* paper including all the other reaction channels
  - final evaluation planned soon

- **Nickel:** $^{56,58,59,60}\text{Ni}(n,p), (n,d), (n,a)$
  - full evaluations 58,59,60 performed in the past
  - new update based on LENZ data underway in collaboration with KAERI

- **Iron:** $^{54,56}\text{Fe}(n,p), (n,d), (n,a)$
  - new update based on LENZ data underway in collaboration with KAERI and BNL

- **Zinc:** $^{64,66}\text{Zn}(n,p), (n,d), (n,a)$
  - under assessment/developing work-plan

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**Experimental data from LENZ:** summing the yield for the $(n,\alpha_0)$ and $(n,\alpha_1)$ reaction channels, shows good agreement with the current ENDF/B-VIII.0 library.
Observation
- Single experiment observations of yield
  - Unpolarized: $\sigma_{\text{tot}}, \sigma, \sigma(\theta)$
  - Polarization:
    - $P_n(E, \theta)$, $A_y(E, \theta)$, $K_x$, ...
    - e.g. $\sigma(^{16}\text{O}(n, n)^{16}\text{O})$,
      $P_n(^{13}\text{C}(\alpha, \bar{n})^{16}\text{O})$

Compilation
- Combination of single-experiment differential data (EXFOR/CSISRS)
- Compound-system data deck
  - e.g.: $^{17}\text{O}(n, n_i)$
  - $^{13}\text{C}(\alpha, \alpha) + ^{13}\text{C}(\alpha, n_i)$
  - $^{16}\text{O}(n, \alpha) + \cdots$
  - RULE: Include all data

Evaluation
- Determination of initial parameters ($E_j, \gamma_{\lambda,c}$) from known/guessed resonance structure (ENSDF, TUNL-NDEP)
- Optimization of
  - $\chi^2 = \sum_{\text{expt}} \chi_{\text{expt}}^2$

Reaction Data
- Energy, angle, energy-angle dependent data formatting
- Formats: ENDF-6, GNDS, etc.

Structure & Decay Data
- Resonance properties: $E_j, \Gamma_{\text{tot},j}, \Gamma_{j,c}, C_{j,c}$
- Formats: RIPL, ENSDF, ANR

Recent LANSCE light-element measurements
- LENZ: $^{12}\text{C}(n, \alpha_0); ^{12}\text{C}(n, p_0); ^{12}\text{C}(n, d_0 + p_1); ^{13}\text{C}(n, \alpha_0): E_n > 7 \text{ MeV}$*
- CoGNAC: $^{12}\text{C}(n, n'\gamma); ^{6}\text{Li}(n, n'\gamma); ^{7}\text{Li}(n, n'\gamma)^*$
- LENZ: $^{16}\text{O}(n, \alpha)$ [See next slide]
- $^{6}\text{Li}(d, n)$: LANSCE personnel, measurement @ Notre Dame

*Pending EDA$_{f90}$ upgrade
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